Dynamics of magnetic nanoparticle with cubic anisotropy in a viscous liquid

N. A. Usov[1-3], M. L. Fdez-Gubieda[1], and J. M. Barandiarán[1]

[1]Departamento de Electricidad y Electrónica, Universidad del País Vasco (UPV/EHU), Apartado 644, 48080 Bilbao, Spain
[2]Institute of Terrestrial Magnetism, Ionosphere and Radio Wave Propagation, Russian Academy of Sciences, (IZMIRAN), 142190, Troitsk, Moscow region, Russia
[3]IKERBASQUE, The Basque Foundation for Science, 48011 Bilbao, Spain
usov@izmiran.ru

Magnetic nanoparticles are important for applications in various areas of nanotechnology, especially for biomedicine [1]. Bacterial magnetosomes are magnetite (Fe_3O_4) nanoparticles with nearly spherical shape. They have a magnetite core of a perfect crystal structure surrounded by a thin lipidic membrane. Magnetosomes are promising for applications in hyperthermia due to their biocompatibility and the very high specific absorption rate (SAR) [2] from high frequency magnetic fields. For a suspension of magnetic nanoparticles in a liquid, both Brownian and Néel relaxation mechanisms may be equally important [3], depending on the particle size, magnetic parameters and liquid viscosity. In the present report, the process of energy absorption from the alternating external magnetic field by a dilute assembly of magnetosomes nanoparticles with cubic type of magnetic anisotropy is studied by means of numerical simulation.

Let $\boldsymbol{n}_1$, $\boldsymbol{n}_2$, $\boldsymbol{n}_3$ be an orthogonal set of the unit vectors that describes the space orientation of one nanoparticle and determines the directions of the easy anisotropy axes of its magnetic anisotropy. The kinematics equations of motion for these vectors are given by

$$\frac{d\vec{n}_i}{dt} = \left[\vec{\omega}, \vec{n}_i\right]; \qquad i = 1 - 3, \tag{1}$$

where $\boldsymbol{\omega}$ is the angular velocity of the particle rotation as a whole, as determined [4] by the corresponding Euler-Langevin stochastic equation

$$I\frac{d\vec{\omega}}{dt} + \xi\vec{\omega} = \vec{N}_m + \vec{N}_{th}, \tag{2}$$

Here I is the moment of inertia of a spherical particle and $\xi = 6\eta V$ is the drag coefficient, η being the dynamic viscosity of the liquid and V being the particle volume. In Eq. (2) $\boldsymbol{N}_m$ is the regular torque due to the external magnetic field acting on the particle, whereas $\boldsymbol{N}_{th}$ is the white noise torque related with the viscous friction forces. It has the following statistical properties [4] ($i,j = x,y,z$)

$$\left\langle N_{th,i}(t)\right\rangle = 0; \qquad \left\langle N_{th,i}(t) N_{th,j}(t_1)\right\rangle = 2k_B T \xi \delta_{ij}\delta(t - t_1), \tag{3}$$

where k_B is the Boltzmann constant and T is the absolute temperature.

The dynamics of the unit magnetization vector of the nanoparticle $\boldsymbol{\alpha}$ is governed [5,6] by the stochastic Landau-Lifshitz equation

$$\frac{\partial\vec{\alpha}}{\partial t} = -\gamma_1\left[\vec{\alpha}, \vec{H}_{ef} + \vec{H}_{th}\right] - \kappa\gamma_1\left[\vec{\alpha}, \left[\vec{\alpha}, \vec{H}_{ef} + \vec{H}_{th}\right]\right], \tag{4}$$

where $\gamma_1 = |\gamma_0|/(1+\kappa^2)$, κ is the damping constant and γ_0 is the gyromagnetic ratio. In Eq. (4) $\boldsymbol{H}_{ef}$ is the effective magnetic field and $\boldsymbol{H}_{th}$ is the thermal field. The latter is assumed to be a Gaussian random process with the following statistical properties for its components [5]

$$\left\langle H_{th,i}(t)\right\rangle = 0; \qquad \left\langle H_{th,i}(t) H_{th,j}(t_1)\right\rangle = \frac{2k_B T\kappa}{|\gamma_0| M_s V}\delta_{ij}\delta(t - t_1). \tag{5}$$

The total energy of a magnetic nanoparticle, with a cubic magnetic anisotropy in the alternating magnetic field $\vec{H}_0 \sin(\omega t)$ reads:

$$W = K_c V\left((\vec{\alpha}\vec{n}_1)^2(\vec{\alpha}\vec{n}_2)^2 + (\vec{\alpha}\vec{n}_1)^2(\vec{\alpha}\vec{n}_3)^2 + (\vec{\alpha}\vec{n}_2)^2(\vec{\alpha}\vec{n}_3)^2\right) - M_s V\vec{\alpha}\vec{H}_0\sin(\omega t), \tag{6}$$

where M_s is the saturation magnetization, K_c is the cubic magnetic anisotropy constant and $\omega = 2\pi f$ is the angular frequency of the applied magnetic field. Using Eq. (6) the effective magnetic field can be calculated as

$$\vec{H}_{ef} = -\frac{\partial W}{V M_s \partial\vec{\alpha}}, \tag{7}$$

whereas the regular torque acting on the particle is given by:

$$\vec{N}_m = \left[\frac{\partial W}{\partial \vec{n}_1}, \vec{n}_1 \right] + \left[\frac{\partial W}{\partial \vec{n}_2}, \vec{n}_2 \right] + \left[\frac{\partial W}{\partial \vec{n}_3}, \vec{n}_3 \right]. \quad (8)$$

In the present paper, calculations of the low frequency hysteresis loops are carried out according to Eqs, (2)-(5) for magnetosome like spherical nanoparticles with saturation magnetization M_s = 480 emu/cm^3 and cubic magnetic anisotropy constant K_c = - 10^5 erg/cm^3. The single domain diameter of a particle having such magnetic parameters is estimated to be D_c = 64 nm. Therefore, the particle diameters are only investigated within the range D = 20 – 60 nm. The dynamic viscosity of a liquid is assumed to be close to that of water, η = 0.01 – 0.1 g/(cm*s). The ranges of magnetic field amplitudes and frequencies considered are typical for magnetic nanoparticle hyperthermia, i.e. H_0 = 30 – 100 Oe and f = 100 – 500 kHz, respectively. To ensure the accuracy of the simulations performed, we use simple Milshtein scheme [6,7] and keep the physical time step lower than 1/50 of the characteristic particle precession time. For every particle diameter a time-dependent particle magnetization $\boldsymbol{M}(t) = \boldsymbol{M_s}\alpha(t)$ is calculated in a sufficiently large series of numerical experiments, N_{exp} = 500 - 1000, for the same frequency and magnetic field amplitude. Because various runs of the calculations are statistically independent, the magnetization of a dilute assembly of nanoparticles is obtained [7] as a correspondent average value, $\langle \boldsymbol{M}(t) \rangle$.

As Fig. 1 shows, in contrast to a uniaxial nanoparticle assembly in a rigid matrix [7], nanoparticles with cubic magnetic anisotropy show hysteresis loops of appreciable squareness even for a low amplitude of the external magnetic field, H_0 = 30 Oe. The loops shown in Fig. 1 correspond to a stationary regime that is achieved after several periods of the alternating magnetic field have been elapsed. The optimal particle diameter for the parameters of Fig 1 is approximately D = 45 nm, and the corresponding SAR value is 207 W/g. It increases greatly as a function of H_0. The dependence of the SAR of a dilute assembly of magnetosomes on the magnetic field parameters H_0 and f, liquid viscosity η and particle diameter D will be fully discussed in the report.

References

[1] Q.A. Pankhurst, N.K.T. Thanh, S.K. Jones, J. Dobson, J. Phys. D: Appl. Phys. **42** (2009) 224001.
[2] R. Herdt, et. al., J. Magn. Magn. Mater. **293** (2005) 80.
[3] R.E. Rosensweig, J. Magn. Magn. Mater. **252** (2002) 370.
[4] W.T. Coffey, Yu.P. Kalmykov, J. Magn. Magn. Mater. **164** (1996) 133.
[5] W.F. Brown, Jr., Phys. Rev. **130** (1963) 1677.
[6] J.L. Garcia-Palacios, F.J. Lazaro, Phys. Rev. B **58** (1998) 14937.
[7] N.A. Usov, J. Appl. Phys. **107** (2010) 123909.

Figures

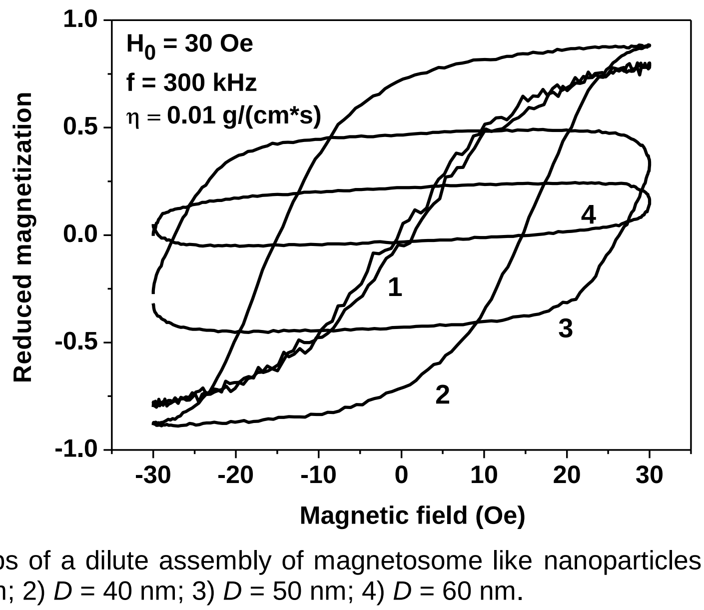

Fig. 1. Hysteresis loops of a dilute assembly of magnetosome like nanoparticles as a function of their diameter: 1) D = 30 nm; 2) D = 40 nm; 3) D = 50 nm; 4) D = 60 nm.